

10/042,522

(FILE 'HOME' ENTERED AT 14:26:16 ON 02 DEC 2003)

FILE 'REGISTRY' ENTERED AT 14:26:22 ON 02 DEC 2003

L1 0 S CL-20/CN  
L2 0 S CL20/CN  
L3 15 S CL-20  
L4 1 S L3 AND HEXA

FILE 'CAPLUS' ENTERED AT 14:28:23 ON 02 DEC 2003

L5 333 S L4  
L6 56 S L5 AND EPSILON  
L7 66714 S INVERSE  
L8 1 S L6 AND L7  
L9 9 S L6 AND CRYSTALLIZATION/IT

FILE 'REGISTRY' ENTERED AT 14:33:31 ON 02 DEC 2003

FILE 'CAPLUS' ENTERED AT 14:34:13 ON 02 DEC 2003

=> s 16 not 19

L10 47 L6 NOT L9

=> d ibib abs hitstr 19 1-9

*applicants*  
D9 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN  
ACCESSION NUMBER: 2003:532386 CAPLUS  
DOCUMENT NUMBER: 139:87406  
TITLE: Inverse solvent-nonsolvent crystallization of HNIW  
(explosive)  
INVENTOR(S): Hamilton, R. Scott  
PATENT ASSIGNEE(S): USA  
SOURCE: U.S. Pat. Appl. Publ., 8 pp.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003130503	A1	20030710	US 2002-42522	20020109
EP 1327633	A1	20030716	EP 2003-250026	20030106
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2003212876	A2	20030730	JP 2003-3320	20030109
PRIORITY APPLN. INFO.:		US 2002-42522	A	20020109

AB Inverse crystn. of the **.epsilon.**-polymorph of  
2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazatetracyclo[5.5.0.05,903,11]  
(HNIW or CL-20) is carried out by adding CL-20 to a dry solvent and adding  
the CL-20-contg. soln. to a non-solvent, which ppts. out the desired CL-20  
polymorph. A basic salt is typically added to neutralize acidic species  
prior to crystn. Suitable crystn. solvents include Et acetate, Me  
acetate, iso-Pr acetate, Bu acetate, THF, and Me Et ketone; suitable  
crystn. non-solvents include hexane, cycloheptane, heptane, octane,  
benzene, toluene, and xylene. CL-20 is preferably synthesized by  
nitration of 2,6,8,12-tetraacetyl-2,4,6,8,10,12-

hexaazatetracyclo[5.5.0.0.05,903,11] (TADA).

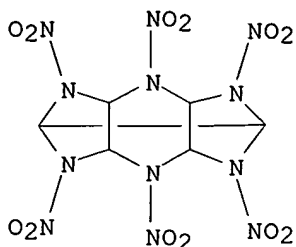
IT **135285-90-4P**

RL: IMF (Industrial manufacture); PRP (Properties); PUR (Purification or recovery); PREP (Preparation)

(inverse solvent-nonsolvent **crystn.** of HNIW (explosive))

RN 135285-90-4 CAPLUS

CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



~~19~~ ANSWER 2 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2002:153686 CAPLUS  
 DOCUMENT NUMBER: 136:202705  
 TITLE: Crystallization of 2,4,6,8,10,12-hexanitro-  
 2,4,6,8,10,12-hexaazatetracyclo[5.5.0.0.05,903,11]-  
 dodecane-an organic oxidizer used as energetic filler  
 in weapons  
 INVENTOR(S): Sanderson, Andrew J.; Hamilton, Richard S.; Warner,  
 Kirstin F.  
 PATENT ASSIGNEE(S): Alliant Techsystems Inc., USA  
 SOURCE: U.S., 6 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6350871	B1	20020226	US 2001-813687	20010321

PRIORITY APPLN. INFO.: US 2000-193468P P 20000331

AB 2,4,6,8,10,12-Hexanitro-2,4,6,8,10,12-hexaazatetracyclo[5.5.0.0.05,903,11]-  
 dodecane (CL-20) is crystd. by dissolving CL-20 in an org. solvent to form  
 a satd. soln., adding a nitrate ester, in which CL-20 is not sol. but  
 which is miscible with the org. solvent, at a nitrate ester to CL-20 wt.  
 ratio of (5-8):1, adding cryst. seeds of the **.epsilon.**-polymorph  
 of Cl-20 to the satd. soln., evapg. the solvent at 25-60.degree.C while  
 growing CL-20 crystals, and removing the nitrate ester and residual  
 solvent from the crystals. The nitrate ester can be poly(glycidyl  
 nitrate), triethyleneglycol-dinitrate, butanetrioltrinitrate, or  
 diglycerol tetranitrate. The org. solvent is preferably Et acetate, but a  
 ketone, a cyclic ether, nitromethane, or acetonitrile can also be used.  
 Cl-20 is an org. oxidizer used as energetic filler in weapons.

IT **135285-90-4P**

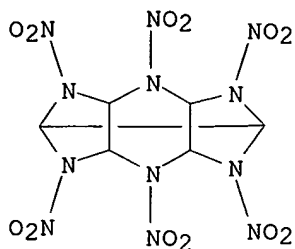
RL: NUU (Other use, unclassified); PEP (Physical, engineering or chemical

process); PUR (Purification or recovery); PYP (Physical process); PREP (Preparation); PROC (Process); USES (Uses)

(**crystn.** of, oxidizer; **crystn.** of 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazatetracyclo[5.5.0.05,903,11]-dodecane-an org. oxidizer used as energetic filler in weapons)

RN 135285-90-4 CAPLUS

CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES. AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 3 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1999:747438 CAPLUS

DOCUMENT NUMBER: 132:4554

TITLE: Crystallization of explosive hexanitrohexaazaisowurtzitane (HNIW) using **epsilon**.-HNIW as seed crystals

INVENTOR(S): Kawabe, Hidefumi; Miya, Hiroshi

PATENT ASSIGNEE(S): Asahi Chemical Industry Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11322752	A2	19991124	JP 1998-148290	19980514
PRIORITY APPLN. INFO.:			JP 1998-148290	19980514

AB In the manuf. of high-d., high-energy, and high-purity **epsilon**.-HNIW from .alpha.-HNIW, .beta.-HNIW, or .gamma.-HNIW by **crystn.**, the starting material is dissolved in a mixed solvent contg. good solvent and poor solvent (whose b.p. is 20.degree. higher than the good solvent), adding **epsilon**.-HNIW crystals into the soln., dropping poor solvent into the soln., and forming **epsilon**.-HNIW by evapg. the solvent. The good solvent is selected from acetone, methylethylketone, THF, and Et acetate, and the poor solvent is selected from toluene and xylene. The **epsilon**.-HNIW is used in the manuf. of explosives.

IT 135285-90-4P, 2,4,6,8,10,12-Hexanitrohexaazaisowurtzitane

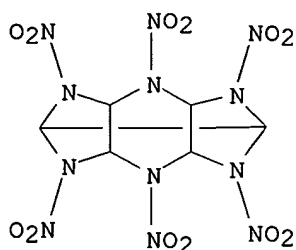
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); PREP (Preparation); PROC (Process)

(**epsilon**.-form; **crystn.** of explosive hexanitrohexaazaisowurtzitane using **epsilon**.-HNIW as seed

crystals)

RN 135285-90-4 CAPLUS

CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



~~19~~ ANSWER 4 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1999:292584 CAPLUS

DOCUMENT NUMBER: 130:298968

TITLE: Antisolvent-solvent crystallization of  
 hexanitrohexaazaisowurtzitane to obtain the .  
**epsilon**.-polymorph

INVENTOR(S): Bescond, Philippe; Graindorge, Herve; Mace, Helene

PATENT ASSIGNEE(S): Societe Nationale des Poudres et Explosifs, Fr.

SOURCE: Eur. Pat. Appl., 12 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 913374	A1	19990506	EP 1998-402636	19981023
EP 913374	B1	20020130		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
FR 2770216	A1	19990430	FR 1997-13546	19971029
FR 2770216	B1	19991203		
US 5973149	A	19991026	US 1998-168413	19981008
NO 9805000	A	19990430	NO 1998-5000	19981027
JP 2000128685	A2	20000509	JP 1998-346525	19981029

PRIORITY APPLN. INFO.: FR 1997-13546 A 19971029

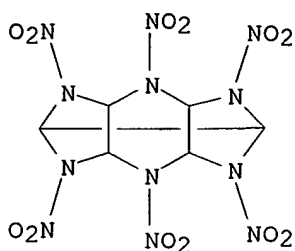
AB A crystn. process for obtaining the .**epsilon**.-polymorph of HNIW (hexanitrohexaazaisowurtzitane) is carried out by: (1) prepg. a satd. soln. of mixed-crystal-morphol. HNIW contg. an org. solvent, selected from a group consisting of esters, nitriles, ethers, and ketones (excluding acetone), and their mixts., and a non-solvent, selected from aliph. and arom. hydrocarbons, and their mixts., in which the solvent for HNIW is more volatile than the non-solvent, (2) seeding the satd. crystal soln. with crystals of the .**epsilon**.-polymorph of HNIW, and (3) concn. of the soln. by evapn., preferably at <50.degree.. The esters are preferably formates and acetates, typically Me acetate, Et acetate, iso-Pr acetate; preferred arom. hydrocarbons are xylenes and toluene.

IT 135285-90-4P, Hexanitrohexaazaisowurtzitane

RL: IMF (Industrial manufacture); PUR (Purification or recovery); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (antisolvent-solvent **crystn.** of hexanitrohexaazaisowurtzitane to obtain the **.epsilon.**-polymorph)

RN 135285-90-4 CAPLUS

CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1999:130417 CAPLUS

DOCUMENT NUMBER: 130:184546

TITLE: Use of chlorine-free non-solvents in solvent crystallization of 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12,-hexaazatetracyclo [5.5.0.05,9.03,11]-dodecane (CL-20) explosive

INVENTOR(S): Johnston, Harold Eugene; Wardle, Robert B.

PATENT ASSIGNEE(S): Cordant Technologies Inc., USA

SOURCE: U.S., 8 pp.  
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5874574	A	19990223	US 1997-991432	19971216
PRIORITY APPLN. INFO.:			US 1997-991432	19971216

AB The high-d. **.epsilon.**-polymorph of cryst. CL-20 (explosive) [2,4,6,8,10,12-hexanitro-2,4,6,8,10,12,-hexaazatetracyclo [5.5.0.05,9.03,11]-dodecane] is isolated by: (1) drying a water-contg. soln. of CL-20 in a solvent, (2) adding a low-d. chlorine-free non-solvent for CL-20 to the dry solvent soln. to induce crystn. and pptn. of the **.epsilon.**-polymorph, (3) sepg. the pptd. **.epsilon.**-CL-20 by adding a polar dense solvent (preferably water) to displace the non-solvent and solvent from the surface of the CL-20 crystals, and (4) recovering the wet CL-20 crystals. An inorg. base can be added to the initial soln. to neutralize any acidic compds. prior to crystn. In addn., a quantity of **.epsilon.**-polymorph CL-20 is added as crystn. seeds. The solvent is chosen from Et acetate, Me acetate, iso-Pr acetate, Bu acetate, THF, and MEK. The chlorine-free non-solvent is typically a hydrocarbon chosen from hexane, cyclohexane, heptane, octane, benzene,

toluene, xylene, hydrocarbon oils, petroleum ether, and ligroine. In this fashion, the **.epsilon.-**polymorph CL-20 is made wet for later handling, packaging, and shipping.

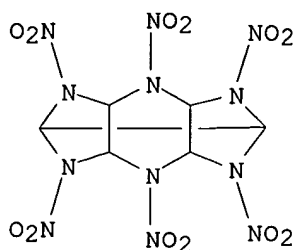
IT 135285-90-4P, 2,4,6,8,10,12-Hexanitro-2,4,6,8,10,12,-hexaazatetracyclo [5.5.0.05,9.03,11]-dodecane

RL: IMF (Industrial manufacture); PUR (Purification or recovery); PREP (Preparation)

(use of chlorine-free non-solvents in solvent **crystn.** of 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12,-hexaazatetracyclo [5.5.0.05,9.03,11]-dodecane (CL-20) explosive)

RN 135285-90-4 CAPLUS

CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~LE~~ ANSWER 6 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN

~~AC~~ ACCESSION NUMBER: 1998:697125 CAPLUS

DOCUMENT NUMBER: 129:316246

TITLE: Preparation of **.epsilon.-**hexanitrohexaazaisowurtzitane as an explosive

INVENTOR(S): Kawanabe, Shushi; Miya, Hiroshi

PATENT ASSIGNEE(S): Asahi Chemical Industry Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10287674	A2	19981027	JP 1997-111756	19970415
JP 2779614	B2	19980723		

PRIORITY APPLN. INFO.: JP 1997-111756 19970415

AB Title compd. (**.epsilon.-I**), useful as an explosive (no data), is prepd. by dissolving I into low-boiling good solvent-poor solvent mixts. and evapg. for **crystn.** **.alpha.-I** in Me<sub>2</sub>CO was mixed with xylene and evapd. to give 92.0% **.epsilon.-I**.

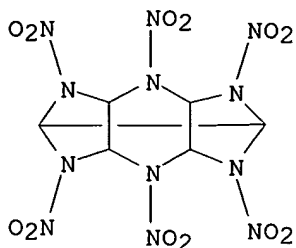
IT 135285-90-4, Hexanitrohexaazaisowurtzitane

RL: PEP (Physical, engineering or chemical process); PROC (Process) (prepn. of **.epsilon.-**hexanitrohexaazaisowurtzitane by **crystn.** from low-boiling solvent mixts.)

RN 135285-90-4 CAPLUS

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CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



~~IS~~ ANSWER 7 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1998:693443 CAPLUS

DOCUMENT NUMBER: 129:316245

TITLE: Preparation of **.epsilon.-**hexanitrohexaazaisowurtzitane using seed crystal

INVENTOR(S): Kawabe, Hidefumi; Miya, Hiroshi

PATENT ASSIGNEE(S): Asahi Chemical Industry Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10287675	A2	19981027	JP 1997-111757	19970415
JP 2893524	B2	19990524		

PRIORITY APPLN. INFO.: JP 1997-111757 19970415

AB Title compd. (**.epsilon.-I**), useful as an explosive (no data), is prepd. by dissolving I into low-boiling good solvent-poor solvent mixts., mixing with **.epsilon.-I** seed crystal, and evapg. for crystn. **.alpha.-I** in Me<sub>2</sub>CO was mixed with PhMe and **.epsilon.-I** seed crystal and evapd. at 3.0-4.0 wt.%/h to give 98.0% **.epsilon.-I**.

IT **135285-90-4**, Hexanitrohexaazaisowurtzitane

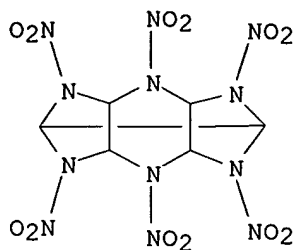
RL: PEP (Physical, engineering or chemical process); PROC (Process)

(prepn. of **.epsilon.-**hexanitrohexaazaisowurtzitane by

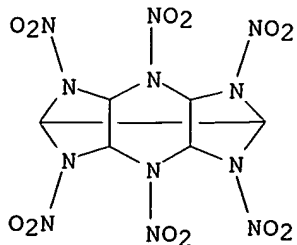
**crystn.** using seed crystal)

RN 135285-90-4 CAPLUS

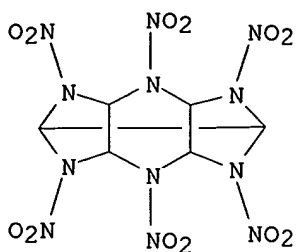
CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



~~13~~ ANSWER 8 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1998:440700 CAPLUS  
 DOCUMENT NUMBER: 129:110953  
 TITLE: Crystallization behavior of hexanitrohexaazaisowurtzitane at 298 K and quantitative analysis of mixtures of its polymorphs by FTIR  
 AUTHOR(S): Kim, Jun-Hyung; Park, Young-Chul; Yim, Yoo-Jin; Han, Jeong-Sik  
 CORPORATE SOURCE: Agency for Defense Development, Taejon, 305-600, S. Korea  
 SOURCE: Journal of Chemical Engineering of Japan (1998), 31(3), 478-481  
 CODEN: JCEJAJ; ISSN: 0021-9592  
 PUBLISHER: Society of Chemical Engineers, Japan  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The crystn. behavior of hexanitrohexaazaisowurtzitane (HNIW) has been investigated at 298 K. Only the .beta. form crystd. at the initial stage of crystn., and it converted to the .epsilon. form with a soln.-mediated transformation mechanism. Through the measurement of the solubilities of each polymorph (.beta. and .epsilon.) at 298 K, it was confirmed that the .epsilon. form is stable and the .beta. form is metastable. In addn., an anal. method has been developed for the detn. of the fraction of the .epsilon. form in the ppts. using a FTIR spectrometer.  
 IT 135285-90-4, Hexanitrohexaazaisowurtzitane  
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)  
 (CL-20; **crystn.** of hexanitrohexaazaisowurtzitane at 298 K and FTIR anal. of its polymorphs)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)







REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1998:424235 CAPLUS

DOCUMENT NUMBER: 129:110410

TITLE: Salting-out process of crystallizing  
2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-  
hexaazatetracyclo[5.5.0.0.5,903,11]dodecane (CL-20)

INVENTOR(S): Johnston, H. Eugene; Wardle, Robert B.

PATENT ASSIGNEE(S): Thiokol Corp., USA; Johnston, H. Eugene; Wardle, Robert B.

SOURCE: PCT Int. Appl., 33 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9827072	A1	19980625	WO 1997-US22298	19971212
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
AU 9853743	A1	19980715	AU 1998-53743	19971212
EP 946527	A1	19991006	EP 1997-950849	19971212
R:	CH, DE, FR, GB, LI, SE			
JP 2001510465	T2	20010731	JP 1998-527767	19971212
NO 9902929	A	19990616	NO 1999-2929	19990616
PRIORITY APPLN. INFO.:			US 1996-33392P	P 19961217
			WO 1997-US22298	W 19971212

AB In the process, CL-20 is dissolved in a mixt. of H<sub>2</sub>O and a solvent for CL-20, e.g., EtOAc, to form 2 liq. phases comprising H<sub>2</sub>O and wet solvent contg. CL-20. The phases are sepd., the CL-20 soln. in the wet solvent is dried by azeotropic distn., a base, e.g., Na<sub>2</sub>CO<sub>3</sub> is added to the dry CL-20 soln. to neutralize acidic species, and a low-d., CL-20 nonsolvent is added to the resulting CL-20 soln. to cause pptn. of **.epsilon**-polymorph CL-20. The CL-20 crystals are sepd. from the nonsolvent and the solvent by adding sufficient H<sub>2</sub>O to displace the nonsolvent and the solvent from the surface of the CL-20 crystals. In this fashion, the .

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**epsilon.**-polymorph CL-20 is made wet for later handling, packaging, and shipping. A schematic presentation of the app. for the process is included.

IT 135285-90-4P, CL-20

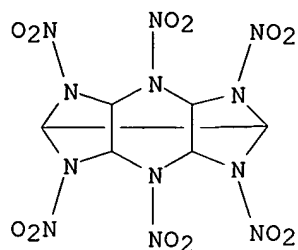
RL: PUR (Purification or recovery); PREP (Preparation)

(**epsilon.**-polymorph; salting-out process of crystg.

2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazatetracyclo[5.5.0.0.5,903,11]  
]dodecane)

RN 135285-90-4 CAPLUS

CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-  
hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

9

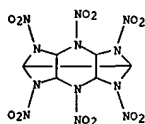
THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> d ibib abs hitstr 110 1-47

10/042,522

110 ANSWER 1 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2003:718354 CAPLUS  
 DOCUMENT NUMBER: 139:325475  
 TITLE: Voids and density distributions in 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane (CL-20) prepared under various conditions  
 AUTHOR(S): Hoffman, D. Mark  
 CORPORATE SOURCE: Energetic Materials Center, Lawrence Livermore National Laboratory, Livermore, CA, 94551, USA  
 SOURCE: Propellants, Explosives, Pyrotechnics (2003), 28(4), 194-200  
 CODEN: PEPYDS; ISSN: 0721-3115  
 PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The d. distributions of six samples of CL-20 were measured by using the d. gradient technique. The technique was used to det. which prepn. procedure produced the highest av. CL-20 d. Assuming crystals with fewer flaws result in reduced sensitivity to shock initiation, higher av. crystal d. (closest to the theor. max. d.) would imply the least no. of voids or inclusions. Based on hot-spot theory, better crystals, i.e., smaller no. of flaws will reduce the shock sensitivity and perhaps other impact initiation mechanisms as well. Six samples from different synthesis and crystn. procedures gave av. densities from 2.042-2.0230 g/cm<sup>3</sup> as measured by d. gradient. Assuming the voids have no d., the crystals were between 99.90-98.98% of the theor. max. d. (TMD for .epsilon.-CL-20 is 2.044 g/cm<sup>3</sup>). An attempt was made to account for the d. difference by identifying voids in the crystals by using polarized light microscopy. This method also gave some insight into the different morphologies produced by different crystn. techniques. In 3 cases voids on the order of several micrometers can be resolved in large CL-20 crystals.  
 IT 135285-90-4P, CL-20  
 RL: IMP (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)  
 (voids and d. distributions in 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane explosive prepd. under various conditions)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)

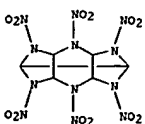


REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

120 ANSWER 2 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2003:284116 CAPLUS  
 DOCUMENT NUMBER: 138:306227  
 TITLE: Synthesis of .epsilon. polymorphic form of a isowurtzitane derivative for explosives and pyrotechnic compositions  
 INVENTOR(S): Cagnon, Guy; Jacob, Guy; Mace, Helene  
 PATENT ASSIGNEE(S): Societe Nationale des Poudres et Explosifs SNPE, Fr.  
 SOURCE: Fr. Demande, 15 pp.  
 CODEN: FRXGBL  
 DOCUMENT TYPE: Patent  
 LANGUAGE: French  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2830533	A1	20030411	FR 1996-3209	19960314
NL 1005411	C2	20030516	NL 1997-1005411	19970303
DE 19710189	A1	20030703	DE 1997-19710189	19970312
ES 2191501	A1	20030901	ES 1997-548	19970313
PRIORITY APPLN. INFO.:			FR 1996-3209	A 19960314

AB The invention relates to polymorphic .epsilon. -hexanitrohexaazaisowurtzitane and its synthesis. According to a 1st variant, hexanitrohexaazaisowurtzitane of an unspecified polymorphic form is mixed in a premixt. contg. 20-40 glycidyl polyazoture and 60-80 wt.% of .gtoreq.1 trinitrate of a monomeric triol contg. 3-12 C atoms. The mixt. is heated in .gtoreq.1 cycle at 40-60.degree. and then at 10-30.degree., and components from the premixt. are eliminated by washing with an org. solvent. According to a 2nd variant, a satd. soln. of hexanitrohexaazaisowurtzitane of an unspecified polymorphic form in an acetone-toluene mixt. is prepd., the soln. is seeded with several crystals of .epsilon.-hexanitrohexaazaisowurtzitane, and the soln. is cond. by evapn. of acetone. Hexanitrohexaazaisowurtzitane, in particular a dense .epsilon.-form, is suitable for explosives or an oxidizing agent used in pyrotechnic compns.  
 IT 135285-90-4P, Hexanitrohexaazaisowurtzitane  
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PNU (Preparation, unclassified); PREP (Preparation); PROC (Process)  
 (synthesis of .epsilon.-hexanitrohexaazaisowurtzitane for explosives and pyrotechnic compns.)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)

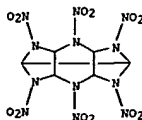


110 ANSWER 1 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

110 ANSWER 3 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2003:117774 CAPLUS  
 DOCUMENT NUMBER: 138:172811  
 TITLE: Low-sensitivity explosives containing CL-20 and plasticized energetic binder  
 INVENTOR(S): Lee, Kenneth E.; Braithwaite, Paul C.; Nicolich, Steve; Mezger, Mark  
 PATENT ASSIGNEE(S): Alliant Techsystems Inc., USA  
 SOURCE: PCT Int. Appl., 28 pp.  
 CODEN: PIXKD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003011797	A2	20030213	WO 2002-US24349	20020731
WO 2003011797	A3	20030424		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BE, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 2003094224	A1	20030522	US 2002-210863	20020731
PRIORITY APPLN. INFO.:			US 2001-309386P	P 20010801

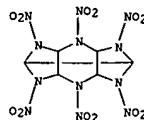
AB A low-sensitivity explosive compn. contains 85-96 wt.% HNIW (CL-20) with av. particle size <30 .mu. (preferably 1-4 .mu.) and 4-15 wt.% of a plasticized binder, comprised of cellulose acetate butyrate and bis(dinitropropyl) acetal/bis(dinitropropyl) formal (BDNPA/P). The explosive has a shock sensitivity of <140 cards, as measured by the NOL Card Gap Test. The prepn. method (i.e., the water/solvent slurry method) is designed to retain and maximize the .epsilon.-CL-20 polymorph.  
 IT 135285-90-4, CL-20  
 RL: FRP (Properties); TEM (Technical or engineered material use); USES (Uses)  
 (explosives contg. low-sensitivity explosives contg. CL-20 and plasticized energetic binder)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



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L10 ANSWER 3 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

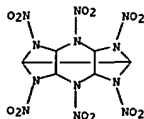
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L10 ANSWER 4 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
ACCESSION NUMBER: 2002:922797 CAPLUS  
DOCUMENT NUMBER: 138:240068  
TITLE: Ageing and service time period assessment of novel solid rocket propellant formulations containing . epsilon.-CL20, AP and energetic plasticizers  
AUTHOR(S): Bohn, Manfred A.  
CORPORATE SOURCE: Fraunhofer-Institut fuer Chemische Technologie, Pfintal-Berghausen, D-76318, Germany  
SOURCE: Proceedings of the International Pyrotechnics Seminar (2001), 28th, 781-795  
CODEN: PPYSD7; ISSN: 0270-1898  
PUBLISHER: Defence Science & Technology Organisation, Pyrotechnics Group  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB To achieve higher burning rates with rocket propellants some batches have been formulated, for which the main ingredients are (1) the energetic plasticizers GAP-A (short chain GAP with azide end groups), TMETN (trimethylol-ethane trinitrate), and BTM (1,2,3-butanetriol trinitrate), (2) the energetic substances ammonium perchlorate (AP) and . epsilon.-CL20 (. epsilon.-HNIV, hexanitro-hexaza-iso-wurtzitane, crystd. in . epsilon.-phase). The binder was GAP-N100. From the point of view of stability and ageing, the interesting fact is that the formulations contain none of the typical stabilizers for the nitric acid ester components TMETN and BTM, although their contents range up to 21 mass %. One reason for doing so is to increase the content of the high energy ingredients. To assess basic stability, a series of tests and investigations were performed. These are the autoignition temp. test (AIT), Dutch mass loss test (DMLT) and vacuum stability test (VST). To investigate ageing, two measurement quantities are used: mass loss as function of time at the temps. of 70, 80, and 90.degree., and heat generation rate as function of time at 70, 80, and 89.degree.. The evaluation of the measurements is based on reaction kinetic models.  
IT 135285-90-4, CL 20  
RL: TEM (Technical or engineered material use); USES (Uses) (ageing and service time period assessment of solid rocket propellant formulations contg. . epsilon.-CL20, ammonium perchlorate and energetic plasticizers)  
RN 135285-90-4 CAPLUS  
CN 5,2,6-(1aimomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS

L10 ANSWER 4 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L10 ANSWER 5 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
ACCESSION NUMBER: 2002:605647 CAPLUS  
DOCUMENT NUMBER: 138:41502  
TITLE: On the kinetics and mechanism of phase transformations in hexanitrohexaazaisowurtzitane. the role of water, microstraining and, dislocations  
AUTHOR(S): Chukanov, N. V.; Raeveskii, A. V.; Golovina, N. I.; Aldoshin, S. M.; Korsounskii, B. L.; Nedelko, V. V.; Dubikhin, V. V.; Volk, F.; Kushnarenko, I. A.  
CORPORATE SOURCE: Institute of Problems of Chemical Physics, Moscow Region, Chernogolovka, 142432, Russia  
SOURCE: International Annual Conference of ICT (2002), 33rd(Energetic Materials), 105/1-105/12  
CODEN: IACIEQ; ISSN: 0722-4087  
PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Kinetics and mechanisms of phase transformations in the crystals of . epsilon.- and . alpha.-modifications of hexanitrohexaazaisowurtzitane were investigated by using optical microscopy, IR spectroscopy, calorimetry and thermogravimetry. The role of water and dislocations at initial stages of the processes is discussed. After completion of the induction period, the phase transition . epsilon.- . gamma. in large crystals is controlled by mech. strains and is accompanied by mech. stimulated chem. decomp. in the front of the phase transition wave.  
IT 135285-90-4, Hexanitrohexaazaisowurtzitane.  
RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses) (effects of water, microstraining and dislocations on kinetics and mechanism of phase transformations in hexanitrohexaazaisowurtzitane)  
RN 135285-90-4 CAPLUS  
CN 5,2,6-(1aimomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



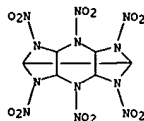
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 6 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2002:540857 CAPLUS  
 DOCUMENT NUMBER: 137:372210  
 TITLE: Kinetic description of mass loss data for the assessment of stability, compatibility and aging of energetic components and formulations exemplified with .epsilon.-CL20  
 AUTHOR(S): Bohn, Manfred A.  
 CORPORATE SOURCE: Fraunhofer-Institut für Chemische Technologie (ICT), Pfintztal, D-76318, Germany  
 SOURCE: Propellants, Explosives, Pyrotechnics (2002), 27(3), 125-135  
 CODEN: PEPYDS; ISSN: 0721-3115  
 PUBLISHER: Wiley-VCH Verlag GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The efficiency of the assessment and of the development of energetic materials can be increased by modeling stability, compatibility, ageing and thermal decompn. of the used components and formulations. All four terms have in common that chem. reactions are the dominating processes, besides for example migration of mobile components. These chem. reactions are only in part controlled by thermodyn., to a great extent they are controlled kinetically. Kinetic models are formulated and used for mass loss measurements with isothermally operated ovens and TGA (thermogravimetric anal.). The models include autocatalytic decompn. and evapn. or decompn. of a minor component beside a main component. A formulation of a general bimol. reaction in terms of mass loss is useful in compatibility studies. Approxns. and simplifications of the autocatalytic models are discussed. The shown applications include new data on hexanitrohexaazaisowurtzitane crystd. in .epsilon.-phase (.epsilon.-HNIW, .epsilon.-CL20) and rocket propellant formulations of type HFK contg. .epsilon.-CL20 as main component. The kinetic data for the decompn. of .epsilon.-CL20 are given and discussed with data from literature.

IT 135285-90-4, CL-20  
 RL: TEM (Technical or engineered material use); USES (Uses) (kinetic description of mass loss data for assessment of stability and compatibility and aging of energetic components and formulations)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(1-iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



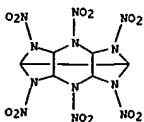
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 7 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2002:510118 CAPLUS  
 DOCUMENT NUMBER: 137:297021  
 TITLE: Morphology prediction and simulation of high energy explosives  
 AUTHOR(S): Han, Yao-Chung; Lee, Woei-Shyong; Lin, Chiu-Hsiung  
 CORPORATE SOURCE: Department of Applied Chemistry, Chung Cheng Institute of Technology, National Defense University, Taiwan  
 SOURCE: Huoyao Jishu (2002), 18(1), 39-61  
 CODEN: HUISE2; ISSN: 1013-767X  
 PUBLISHER: Society of Explosives and Propellants  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Chinese

AB The aim of this study is to simulate the dynamic crystal morphol. of HNIW and ONC, the advanced high-energy explosives. The UFF, the DREIDING and the COMPASS mol. forces fields, resp., assocd. with Bravais-Friedel-Donnay-Harker (BFDH) and attachment habit theories were used in the mol. simulations. The computational results of the attachment and the slice energies of the crystal primary faces have shown that the .epsilon.-HNIW explosive has less attachment energies and much easier to explode so that it can be used as the warhead's main charge for military purposes. The predictions of the slice energies have concluded that the thermal stability of the ONC explosive is higher than that of the HNIW explosive. The packing d. of the ONC explosive is 2.111 kg/m3, which was estd. using the Compass mol. force field and was the highest value among the synthesized explosives.

IT 135285-90-4, HNIW  
 RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses) (simulation of dynamic crystal morphol. of high energy explosives)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(1-iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



L10 ANSWER 6 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

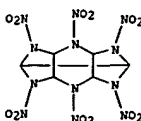
L10 ANSWER 8 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2002:487940 CAPLUS  
 DOCUMENT NUMBER: 137:65360  
 TITLE: Preparation of low-energy-initiated CL-20 explosive by coating of crystals with polymeric binders  
 INVENTOR(S): Chan, May L.; Bui-Dang, Que Thingoc; Hennings, George N.; Reynolds, Thomas Lee; Reynolds, Richard Kent; Ladika, Michael Damon  
 PATENT ASSIGNEE(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 6 pp., Division of U. S. Ser. No. 513,035.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

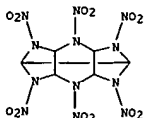
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002079030	A1	20020627	US 2001-2894	20011205
PRIORITY APPLN. INFO.:			US 2000-513035	A3 20000225

AB An explosive suitable for low-energy initiation is prepd. by coating .epsilon.-CL-20 crystals (1-5 .mu. size) with 1-3 wt.% of a polymeric binder. The polymer binder is selected from polyethyl acrylate, Et acrylate-Bu acrylate copolymer, acrylic polystyrene resin, fluoropolymers, vinyl acetate-ethylene copolymer, vinyl chloride-vinyl acetate copolymer, ethylene-vinyl chloride copolymer, acrylic polymers, polyester-polyurethanes, vinyl acetate-dibutyl maleate copolymer, vinyl acetate-dibutyl maleate-acrylic terpolymer, styrene-butadiene-itaconic acid copolymer, vinylidene chloride-Me methacrylate-acrylonitrile copolymer, vinyl acetate-Bu acrylate copolymer, polyvinyl versate, and vinylpyrrolidone-styrene copolymer. The explosive is coated by either a slurry method or by using a nonaq. liq. to suspend CL-20 and adding the polymer binder. Such explosives are useful in the fabrication of exploding foil initiators for military ordnance.

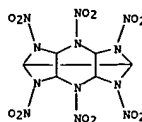
IT 135285-90-4, CL-20  
 RL: PEP (Physical, engineering or chemical process); PYP (Physical process); TEM (Technical or engineered material use); PROC (Process); USES (Uses) (coating of; prepn. of low-energy-initiated CL-20 explosive by coating of crystals with polymeric binders)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(1-iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



~~110~~ ANSWER 9 OF 47 CAPIUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2001:618703 CAPIUS  
 DOCUMENT NUMBER: 135:290896  
 TITLE: Theoretical studies on the structures and properties of hexanitrohexaazaisowurtzitane  
 AUTHOR(S): Zhang, Ji; Xiao, He-Ming; Ji, Guang-Fu  
 CORPORATE SOURCE: Dep. Chem., Nanjing Univ. of Science and Technol., Nanjing, 210094, Japan  
 SOURCE: Ruixue Xuebao (2001), 59(8), 1265-1271  
 CODEN: HHHPA4; ISSN: 0567-7351  
 PUBLISHER: Kexue Chubanshe  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Chinese  
 AB The mol. geometries, electronic structures, IR spectra and thermodyn. properties at 298-1000 K range of .alpha.(.gamma.), .beta., and .epsilon.-conformations of hexanitrohexaazaisowurtzitane (HNHW) are calcd. by using ab initio and d. functional theory (DFT) methods at HF/6-31G\* and B3LYP/6-31G\* level, resp. The results obtained from the two methods have been carefully compared with each other and with the exptl. data. The optimized parameters of geometry are in good agreement with the exptl. values. Compared with the other bonds in HNHW, the bond lengths of N-N are longer and Mulliken population of N-N is smaller, which means that the N-N may be the initial bond in pyrolysis and explosion. The obtained IR spectra are also in good accordance with the exptl. results and the av. abs. difference is < 45 cm<sup>-1</sup>. The thermodyn. stability order [.epsilon.] > [.alpha.(.gamma.)] > [.beta.] predicted from frontier MO energies and their gaps is the same as that measured from expts.  
 IT 135285-90-4, Hexanitrohexaazaisowurtzitane  
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); TEM (Technical or engineered material use); PROC (Process); USES (Uses) (theor. detn. of structures and properties of hexanitrohexaazaisowurtzitane)  
 RN 135285-90-4 CAPIUS  
 CN 5,2,6-(1minomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)

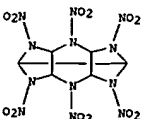


~~110~~ ANSWER 10 OF 47 CAPIUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2001:605162 CAPIUS  
 DOCUMENT NUMBER: 135:325421  
 TITLE: Solvent effects on the morphology of .epsilon.-CL-20 crystals  
 AUTHOR(S): Thoms, Volker; Kempa, Paul Bernd; Herrmann, Michael  
 CORPORATE SOURCE: Fraunhofer ICT, Berghausen, 76327, Germany  
 SOURCE: International Annual Conference of ICT (2001), 32nd(Energetic Materials), 157/1-157/7  
 CODEN: IACIEQ; ISSN: 0722-4087  
 PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A no. of solvents were tested on influencing the morphol. of .epsilon.-CL-20 crystals. The examples of diisopropyl ether, Me iso-Bu ketone, nitrobenzene and H2O show that different morphologies of .epsilon.-CL-20 are found after recrystn. Solvents affect crystal growth of CL-20 from soln. and change the morphologies of .epsilon.-CL-20. This fact is very important for handling CL-20 like filtrating, grinding or storage, because the mech. stability depends on the shape of the crystals. X-ray diffraction patterns of the crystals were analyzed with Rietveld refinement to find out the texture of the faces and the preferred growth directions of the crystals. SEM pictures show that in some cases the blocking of energetically favorable sites by solvent mols. creates odd-looking morphologies.  
 IT 135285-90-4, CL-20  
 RL: PRP (Properties)  
 (solvent effects on morphol. of .epsilon.-CL-20 crystals)  
 RN 135285-90-4 CAPIUS  
 CN 5,2,6-(1minomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



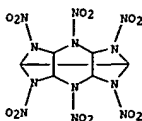
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~110~~ ANSWER 11 OF 47 CAPIUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2001:605158 CAPIUS  
 DOCUMENT NUMBER: 135:259344  
 TITLE: Stability and service time period assessment of novel solid rocket propellant formulations containing CL20, AP and energetic plasticizers  
 AUTHOR(S): Bohn, Manfred A.; Eisele, Siegfried  
 CORPORATE SOURCE: Fraunhofer-Institut fuer Chemische Technologie (ICT), Pfintal-Berghausen, D-76318, Germany  
 SOURCE: International Annual Conference of ICT (2001), 32nd(Energetic Materials), 152/1-152/13  
 CODEN: IACIEQ; ISSN: 0722-4087  
 PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 AB To achieve higher burning rates with rocket propellants some batches were formulated, for which the main ingredients are the energetic plasticizers GAP-A, TMETN (trimethylolethane trinitrate) and BTNN (1,2,3-butanetriol trinitrate), the energetic substances ammonium perchlorate and .epsilon.-CL20 (.epsilon.-HNHW). The binder was GAP-N100. From the view of stability, the interesting fact is that the formulations contain no typical stabilizer for the nitric acid ester components TMETN and BTNN, although their contents range .ltoreq.21 mass%. One reason to do this is to increase the content of the high energy substances. To assess the stability and aging a series of tests and investigations was performed. These were Dutch Mass Loss Test, Vacuum Stability Test, mass loss as function of time at the temps. of 80 and 90.degree., and heat generation rate measurements as function of time at 80.degree. with the Thermal Activity Monitor of Thermometric AB, Sweden. The evaluation of the measurements is based on kinetic models.  
 IT 135285-90-4  
 RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses) (stability and service time period assessment of novel solid rocket propellant formulations contg. CL20, AP, and energetic plasticizers)  
 RN 135285-90-4 CAPIUS  
 CN 5,2,6-(1minomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



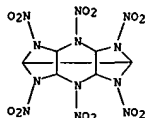
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~110~~ ANSWER 12 OF 47 CAPIUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2001:605115 CAPIUS  
 DOCUMENT NUMBER: 135:311219  
 TITLE: Phase transformations in hexanitrohexaazaisowurtzitane  
 AUTHOR(S): Chukanov, N. V.; Golovina, N. I.; Nedelko, V. V.; Dubikhin, V. V.; Voschikova, S. A.; Anan'ina, O. A.; Larikova, T. S.; Nazin, G. M.; Aldoshin, S. M.; Korsounskii, B. L.; Volk, F.  
 CORPORATE SOURCE: Institute of Problems of Chemical Physics, Russian Academy of Sciences, Chernogolovka, 142432, Russia  
 SOURCE: International Annual Conference of ICT (2001), 32nd(Energetic Materials), 101/1-101/9  
 CODEN: IACIEQ; ISSN: 0722-4087  
 PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Using IR spectroscopy, calorimetry, and x-ray anal. the structure and phase transitions of .alpha.- and .epsilon.-modifications of hexanitrohexaazaisowurtzitane into .gamma.-form were studied. The transition .alpha.-.fwdarw..gamma. proceeds with self-acceleration. Apparently, this is caused by topochem. nature of the process, including nucleation and frontal propagation. The poor reproducibility of the results is characteristic for the transition .epsilon.-.fwdarw..gamma. in polycryst. sample. The process has essentially discrete nature, which may be explained by the dependence of the ability of the crystals to undergo phase transition on their morphol., particularly, on the defects in the crystals. Cooperative effect is characteristic for this process. This effect is caused by the ability of phase transition in one crystal to induce the resp. transitions in the whole cluster of adjacent crystals.  
 IT 135285-90-4, Hexanitrohexaazaisowurtzitane  
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process) (crystal structure and phase transition of)  
 RN 135285-90-4 CAPIUS  
 CN 5,2,6-(1minomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



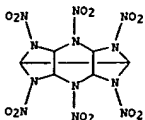
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~13~~ ANSWER 13 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2001:476854 CAPLUS  
 DOCUMENT NUMBER: 135:228932  
 TITLE: Thermal decomposition of various modifications of hexanitrohexaazaisowurtzitane  
 AUTHOR(S): Nedelko, V. V.; Chukanov, N. V.; Golovina, N. I.; Korsounskii, B. L.; Larikova, T. S.; Volk, F.  
 CORPORATE SOURCE: Institute of Problems of Chemical Physics, Russian Academy of Sciences, Chernogolovka, 142432, Russia  
 SOURCE: New Trends in Research of Energetic Materials, Proceedings of the Seminar, 4th, Pardubice, Czech Republic, Apr. 11-12, 2001 (2001), 257-263.  
 Editor(s): Zeman, Svatopluk. University of Pardubice: Pardubice, Czech Rep.  
 CODEN: 69BKIC  
 DOCUMENT TYPE: Conference  
 LANGUAGE: English  
 AB The thermal decompn. of .alpha.-, .beta.-, .gamma.-, and .epsilon.-hexanitrohexaazaisowurtzitane (HNW) is investigated by thermogravimetry, IR-spectroscopy, optical microscopy and X-ray diffractometry. At the earliest stages of decompn. (.ltoreq. 0.1t) .alpha.-, .beta.-, and .epsilon.-HNW undergo the thermal phase transitions into .gamma.-form. The kinetics of decompn. depends on the particle size and crystal morphol. Decompn. kinetic law of a HNW polymorph is detd. by its crystal nature. Even the very small quantities of water in .epsilon.-HNW (up to 0.1 wt. %) det. the structure of crystal and cause the growth of the elementary cell parameters. This phenomenon affects the decompn. kinetics.  
 IT 135285-90-4, Hexanitrohexaazaisowurtzitane  
 RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)  
 (deth. of thermal decompn. of various modifications of hexanitrohexaazaisowurtzitane by thermogravimetry and IR-spectroscopy and optical microscopy and X-ray diffractometry)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



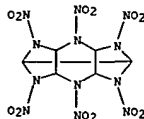
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~15~~ ANSWER 15 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2001:279522 CAPLUS  
 DOCUMENT NUMBER: 134:282928  
 TITLE: Water slurry-coating method for manufacture of pressable and extrudable CL-20-based explosive formulations  
 INVENTOR(S): Lee, Kenneth E.; Hatch, Robert L.; Braithwaite, Paul  
 PATENT ASSIGNEE(S): Cordant Technologies Inc., USA  
 SOURCE: U.S., 9 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:  
 PATENT NO. KIND DATE APPLICATION NO. DATE  
 US 6217799 B1 20010417 US 1998-166843 19981006  
 PRIORITY APPLN. INFO.: US 1997-61236P P 19971007  
 AB Pressable or extrudable explosive formulations based on CL-20 are prepd. by a water slurry method consisting of: (1) prepg. an aq. dispersion of CL-20 (.epsilon.-polymorph), (2) mixing into the dispersion a plasticizer, a lacquer contg. a non-energetic binder, and a solvent, and (3) agitating the slurry and removing the solvent to form coated granules. The mixing and agitating steps are carried out at a sufficiently low temp. and the solvent is present at a suitable low temp., such as to avoid polymorph conversion of the .epsilon.-polymorph of CL-20. The coated granules consist of 85-96 wt.1. CL-20, and may also contain a stabilizer (selected from diphenylamine and N-alkylnitroanilines). The formulation can be formed into explosive grains suitable for ordnance, such as grenades, land mines, missile warheads, and demolition explosives.  
 IT 135285-90-4, CL-20  
 RL: PEP (Physical, engineering or chemical process); TEM (Technical or engineered material use); PROC (Process); USES (Uses)  
 (explosives; water slurry-coating method for manuf. of pressable and extrudable CL-20-based explosive formulations)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)

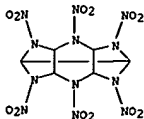


REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~14~~ ANSWER 14 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2001:285136 CAPLUS  
 DOCUMENT NUMBER: 134:369069  
 TITLE: New high explosive - polycyclic nitramine hexanitrohexaazaisowurtzitane (HNW, CL-20)  
 AUTHOR(S): Andelkovic-Lukic, Mirjana  
 CORPORATE SOURCE: Tehnicki opitni centar, Belgrade, 11000, Yugoslavia  
 SOURCE: Naucno-Tehnicki Pregled (2000), 50(6), 60-64  
 CODEN: NPGLA7; ISSN: 0350-0667  
 PUBLISHER: Vojnotehnicki Institut VJ  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Serbian  
 AB Physico-chem. and detonation properties of a new high explosive are presented and compared with octogen. CL-20 exists in four cryst. forms, stable at different temps. Only the .epsilon. and the .beta. form are used in exploitation. CL-20 has better detonation properties than octogen, higher d. and detonation rate but lower impact and friction sensitivity (of the PETN class). The CL-20 m.p. is lower than in octogen, 240.degree..  
 IT 135285-90-4, CL-20  
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); TEM (Technical or engineered material use); PROC (Process); USES (Uses)  
 (detonation properties of CL-20)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)

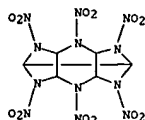


~~16~~ ANSWER 16 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2001:69500 CAPLUS  
 DOCUMENT NUMBER: 134:282873  
 TITLE: Study on decomposition and impact sensitivity of .epsilon.-hexanitrohexaazaisowurtzitane in three particle sizes  
 AUTHOR(S): Xu, Yongjiang; Jin, Shaohua; Ou, Yuxiang; Song, Quancai  
 CORPORATE SOURCE: Beijing Institute of Technology, Beijing, 100081, Peop. Rep. China  
 SOURCE: Huozhayao Xuebao (2001), 24(1), 47-48, 46  
 CODEN: HUXUPP  
 PUBLISHER: Zhongguo Bingqi Gongye Di-204 Yanjiusuo  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Chinese  
 AB The thermal decompn. of .epsilon.-hexanitrohexaazaisowurtzitane (.epsilon.-HNW) in three particle sizes was studied by DTA, and the formal kinetic parameters E and A were obtained. The impact sensitivity of .epsilon.-HNW corresponding to particle sizes was detd. The effect of particle size on the formal kinetic parameters and impact sensitivity of .epsilon.-HNW was discussed.  
 IT 135285-90-4  
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); TEM (Technical or engineered material use); PROC (Process); USES (Uses)  
 (decompn. and impact sensitivity of .epsilon.-hexanitrohexaazaisowurtzitane in three particle sizes)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



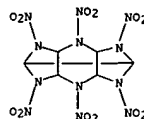


~~L10~~ ANSWER 17 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2001:45351 CAPLUS  
 DOCUMENT NUMBER: 134:133763  
 TITLE: Theoretical study on pyrolysis initiation reactions of hexanitrohexaazaisowurtzitane in gas phase  
 AUTHOR(S): Zhang, Ji; Xiao, He-ming; Gong, Xue-dong; Li, Jin-zhan  
 CORPORATE SOURCE: Department of Chemistry, Nanjing University of Science and Technology, Nanjing, 210094, Peop. Rep. China  
 SOURCE: Hanneng Cailliao (2000), 8 (4), 149-154  
 CODEN: HACAQJ; ISSN: 1006-9941  
 PUBLISHER: Hanneng Cailliao Bianjibu  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Chinese  
 AB The quantum-chem. UHF-SCF-PM3 MO method was employed to calc. the pyrolysis initiation reactions of .alpha., .beta., .gamma., .epsilon. and .delta. polymorphs of hexanitrohexaazaisowurtzitane in gas phase. Their transition states, activation energies, and potential energy curves have been obtained. The changes of the geometries, energies and at. charges over these reactions are revealed. The mechanism of pyrolysis initiation reaction of titled compd. is similar to that of usual non-caged nitramine explosives. In addn., the relation between the activation energy and the impact sensitivity is also discussed.  
 IT 135285-90-4, Hexanitrohexaazaisowurtzitane  
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); TEM (Technical or engineered material use); PROC (Process); USES (Uses) (anal. of pyrolysis initiation reactions of hexanitrohexaazaisowurtzitane polymorphs in gas phase)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)

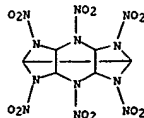


L10 ANSWER 18 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)  
 REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~L10~~ ANSWER 18 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2000:832052 CAPLUS  
 DOCUMENT NUMBER: 134:6628  
 TITLE: Comparative investigation of thermal decomposition of various modifications of hexanitrohexaazaisowurtzitane (CL-20)  
 AUTHOR(S): Nedelko, V. V.; Chukanov, N. V.; Raevskii, A. V.; Korsounskii, B. L.; Larikova, T. S.; Kolesova, O. I.; Volk, F.  
 CORPORATE SOURCE: Institute of Problems of Chemical Physics, Russian Academy of Sciences, Chernogolovka, 142432, Russia  
 SOURCE: Propellants, Explosives, Pyrotechnics (2000), 25 (5), 255-259  
 CODEN: PEPYD5; ISSN: 0721-3115  
 PUBLISHER: Wiley-VCH Verlag GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The thermal decompn. kinetics of different polymorphs of CL-20 (.alpha., .gamma. and .epsilon.) was investigated by thermogravimetry, IR spectroscopy, and optical and electronic microscopy. The reactions proceed with self-acceleration and can be described by a kinetic law of first order with autocatalysis. Already at the earliest stages of decompn. (.ltoreq. 1%) phase transitions take place from .alpha. .fwdarv. .gamma. and from .epsilon. .fwdarv. .gamma.. For this reason the obsd. decompn. is related to the decompn. of .gamma.-CL-20. On the other hand, the kinetics of decompn. depends on the initial polymorphic state, so that the thermal decompn. increases in the series: .alpha. < .gamma. < .epsilon.. Expts. with different samples of .alpha.-CL-20 demonstrate that different rates of decompn. are obsd. for the same polymorph depending on the mean size and the size distribution of the crystals and their morphol. features. In some cases the thermal stability of .alpha.-CL-20 can be increased by previous annealing. The thermal decompn. of CL-20 is purely a solid-state process. Microscopical and spectroscopical anal. of the condensed CL-20 decompn. product (formed after prolonged heating at high temp.) show that it has a network structure and consists mainly of carbon and nitrogen.  
 IT 135285-90-4, Hexanitrohexaazaisowurtzitane  
 RL: RCT (Reactant); TEM (Technical or engineered material use); RACT (Reactant or reagent); USES (Uses) (comparative anal. of thermal decompn. kinetics of polymorphs of hexanitrohexaazaisowurtzitane)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)

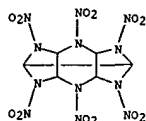


~~L10~~ ANSWER 19 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2000:581210 CAPLUS  
 DOCUMENT NUMBER: 133:195549  
 TITLE: Polymorphism and solubility of CL20 in plasticizers and polymers  
 AUTHOR(S): Torry, Simon; Cunliffe, Anthony  
 CORPORATE SOURCE: DERA, Kent, TN14 7BP, UK  
 SOURCE: International Annual Conference of ICT (2000), 31st (Energetic Materials), 107/1-107/12  
 CODEN: IACTEQ; ISSN: 0722-4087  
 PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The most powerful com. available explosive, 2,4,6,8,10,12-hexanitro hexaazaisowurtzitane (CL20) can exist in at least 4 phases. The preferred polymorph is the .epsilon. phase as it is morphol. stable at room temp. and has the highest d. of the CL20 polymorphs. The CL20 soly. and the rate of polymorph conversion at various temps. in different plasticizers and polymers were investigated. Soly. was measured using variable temp. proton NMR spectroscopy. The rate of polymorph conversion was quantified by partial least squares anal. of IR spectroscopy data. CL20 polymorph conversion was found to be a complex process. There was evidence that 1:1 mixes of .epsilon.- and .gamma.-CL20 obeyed Ostwald's rule of stages. At temps. above the .epsilon.- to .gamma.-phase transition, the metastable .epsilon.-polymorph was formed in excess before it converted into the stable .gamma.-phase. The .epsilon.- to .gamma.-phase transition temp. was estd. to be 56.5+-1.5.degree.C.  
 IT 135285-90-4, CL20  
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); TEM (Technical or engineered material use); PROC (Process); USES (Uses) (polymorphism and soly. of CL20 in plasticizers and polymers)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



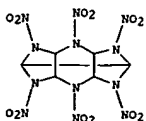
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 20 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2000:581099 CAPLUS  
 DOCUMENT NUMBER: 133:179879  
 TITLE: Exploring of interactions of the nitramines HMX and CL20 with components in formulations by computer simulation  
 AUTHOR(S): Thoma, V.; Kempa, P. B.; Bohn, M. A.  
 CORPORATE SOURCE: Fraunhofer-Institut für Chemische Technologie, ICT, Pfintal-Berghausen, D-76318, Germany  
 SOURCE: International Annual Conference of ICT (2000), 31st (Energetic Materials), 63/1-63/19  
 CODEN: IACIEQ; ISSN: 0722-4087  
 PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 AB The development of a methodical determinative model was discussed for prediction of potential intermol. interactions of candidate energetic formulations, based on semiempirical quantum chem. calcns. The compds. in question were cryst. .beta.-HMX, and .epsilon.-CL20; reactive formulation components were the energetic binder GAP (glycidyl azide polymer) and guanidine as a carrier for NH2-groups. Reactive configurations were given to analyze bond length changes for the interactions of .beta.-HMX and .epsilon.-CL20 with GAP and guanidine. For GAP, the representative chain length was used for the simulation. Guanidine was comparably reactive for both HMX cryst. forms, although there was a higher tendency for reaction with .epsilon.-CL20. According to the criteria, GAP and .epsilon.-CL20 showed a high reactivity in comparison with .beta.-HMX. The pos. partial charge of the H atom was, on av., greater with .epsilon.-CL20 than with .beta.-HMX, in which it was assumed that at least one C atom in the CH-CH-group in .epsilon.-CL20 was more pos., which favored the H-cleavage reaction for .epsilon.-CL20, compared with .beta.-HMX.  
 IT 135285-90-4, CL-20  
 RI: PRP (Properties)  
 (systems) modeling of mol. interactions of nitramines with amine and azide components in energetic formulations)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (SCI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

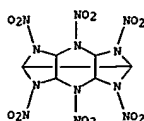
ANSWER 21 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2000:580918 CAPLUS  
 DOCUMENT NUMBER: 133:195542  
 TITLE: Comparative investigation of thermal decomposition of various modifications of hexanitrohexaazaisowurtzitane  
 AUTHOR(S): Nedelko, V. V.; Chukanov, N. V.; Korsounskii, B. L.; Larikova, T. S.; Volk, F.  
 CORPORATE SOURCE: Institute of Problems of Chemical Physics, Russian Academy of Sciences, Moscow Region, 142432, Russia  
 SOURCE: International Annual Conference of ICT (2000), 31st (Energetic Materials), 9/1-9/9  
 CODEN: IACIEQ; ISSN: 0722-4087  
 PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The thermal decompn. of .alpha.-, .gamma.- and .epsilon.-hexanitrohexaazaisowurtzitane (HNW) has been investigated by manometric, thermogravimetric, IR-spectroscopic and microscopic methods. Kinetic parameters of the reactions have been detd. in terms of the first-order autocatalysis equation. The .alpha.-Form of HNW has lowered thermal stability as compared with .gamma.- and .epsilon.-forms. The complete thermal phase transitions of .alpha.- and .epsilon.-polymorphs into .gamma.-HNW occur already at low decompn. conversions (up to 1%), thus the obsd. difference in the kinetic behavior should be explained by phys. reasons such as morphol., particle size, concn. of defects.  
 IT 135285-90-4, HNW  
 RI: RCT (Reactant); TEM (Technical or engineered material use); RACT (Reactant or reagent); USES (Uses)  
 (comparative investigation of thermal decompn. of various modifications of hexanitrohexaazaisowurtzitane)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (SCI) (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

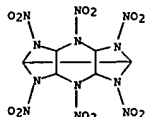
L10 ANSWER 20 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

ANSWER 22 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2000:353862 CAPLUS  
 DOCUMENT NUMBER: 132:349809  
 TITLE: New aspects of the impact reactivity of nitramines  
 AUTHOR(S): Zeman, Svatopluk  
 CORPORATE SOURCE: Department of Theory and Technology of Explosives, University of Pardubice, Pardubice, CZ-532, Czech Rep.  
 SOURCE: Propellants, Explosives, Pyrotechnics (2000), 25(2), 66-74  
 CODEN: PEPYDS; ISSN: 0721-3115  
 PUBLISHER: Wiley-VCH Verlag GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The impact reactivity ("the first reaction") of nitramines was detd. as the drop energy Ed, required for 50% initiation probability. Relationships were found between the Ed values, on the one hand, and heats of fusion, 15W NMR chem. shifts of azo atoms in reaction centers, parameters of low-temp. thermolysis, and oxygen balances of nitramines studied, on the other. Taking these relationships the Ed values were predicted for 4 nitramines, from which 3 were not synthesized yet. On the basis of the said relationships it was stated that the impact reactivity of nitramine mols. depends on the electronic configuration within their reaction centers and on their conformational stability and intensity of their intermol. interactions. The reaction centers here are the same as in the case of initiation of the nitramines by shock. It is found that .epsilon.-HNW possesses higher thermal and impact reactivities in comparing with those of .beta.-modification.  
 IT 135285-90-4, HNW  
 RI: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)  
 (impact reactivity of nitramines)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (SCI) (CA INDEX NAME)

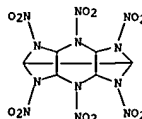


REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

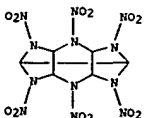
L10 ANSWER 23 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2000:344850 CAPLUS  
 DOCUMENT NUMBER: 133:45723  
 TITLE: Quantitative analysis of mixture of .epsilon.  
 .-HNIV and .gamma.-HNIV  
 AUTHOR(S): Gao, Haiyan; Zhang, Yunhong; Yin, Penggang  
 CORPORATE SOURCE: Fire-retarded Laboratory, Beijing University of  
 Science and Technology, Beijing, 100081, Peop. Rep.  
 China  
 SOURCE: Huozhayao Xuebao (2000), 23(2), 62-63  
 CODEN: HUXUFF  
 PUBLISHER: Zhongguo Bingqi Gongye Di-204 Yanjiuso  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Chinese  
 AB A method of quant. anal. of mixt. of .epsilon.-HNIV and  
 .gamma.-HNIV by FT-IR was given. The peaks within 832.39-819.312 cm-1  
 were used as the basis of quant. anal.  
 IT 135285-90-4, HNIV  
 RL: PEP (Physical, engineering or chemical process); FRP (Properties); TEM  
 (Technical or engineered material use); PROC (Process); USES (Uses)  
 (quant. anal. of mixt. of .epsilon.-HNIV and .gamma.-HNIV)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(1minomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-  
 hexanitro- (9CI) (CA INDEX NAME)



L10 ANSWER 24 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2000:344849 CAPLUS  
 DOCUMENT NUMBER: 133:76151  
 TITLE: Determination of crystal density of four polymorphs of  
 hexanitrohexaazaisowurtzitane (HNIV)  
 AUTHOR(S): Ou, Yuxiang; Xu, Yongjiang  
 CORPORATE SOURCE: Beijing University of Science and Technology, Beijing,  
 100081, Peop. Rep. China  
 SOURCE: Huozhayao Xuebao (2000), 23(2), 60-61, 59  
 CODEN: HUXUFF  
 PUBLISHER: Zhongguo Bingqi Gongye Di-204 Yanjiuso  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Chinese  
 AB The crystal d. (p and pm) of four polymorphs (.alpha.-HNIV/2H2O,  
 .beta.-HNIV, .gamma.-HNIV and .epsilon.-HNIV) of HNIV was  
 obtained. The pc was calcd. according to crystal parameters given by  
 X-ray diffractometers. The pm was detd. according to d. bottle method  
 defined by GJB772A-97, 401.1. The pc values were 1.992, 1.989, 1.918, and  
 2.044 g/cm3 resp. and the pm values were 1.937, 1.983, 1.918, and 2.035  
 g/cm3 resp. The pcs were 0.055, 0.006, 0, and 0.009 g/cm3 resp., higher  
 than pm.  
 IT 135285-90-4, Hexanitrohexaazaisowurtzitane  
 RL: PEP (Physical, engineering or chemical process); FRP (Properties); TEM  
 (Technical or engineered material use); PROC (Process); USES (Uses)  
 (deta. of crystal d. of polymorphs of hexanitrohexaazaisowurtzitane)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(1minomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-  
 hexanitro- (9CI) (CA INDEX NAME)



L10 ANSWER 25 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1999:726251 CAPLUS  
 DOCUMENT NUMBER: 131:339055  
 TITLE: Analytical characterization of impurities or  
 byproducts in new energetic materials  
 AUTHOR(S): Bunte, Gudrun; Pontius, Heike; Kaiser, Manfred  
 CORPORATE SOURCE: Fraunhofer-Institut für Chemische Technologie (ICT),  
 Pfingst-Berghausen, D-76327, Germany  
 SOURCE: Propellants, Explosives, Pyrotechnics (1999), 24(3),  
 149-155  
 CODEN: PEPYDS; ISSN: 0721-3115  
 PUBLISHER: Wiley-VCH Verlag GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB In the last years several new explosives have recently attracted attention  
 as possible alternatives, e.g. for the nitramines RDX and HMX.  
 Hexanitrohexaazaisowurtzitane (HNIV) also known as CL 20 is one of them.  
 Objective of the study was to analyze three different CL 20 samples from  
 different suppliers (.epsilon.-CL 20 from Thiokol, USA and .  
 epsilon.- and .beta.-CL 20 from SNPE, France) with chromatog. and  
 spectroscopic techniques to characterize the chem. and polymorph purity of  
 the materials in order to compare the different samples to each other.  
 From IR-spectroscopic measurements it was detd. that all three materials  
 have polymorph purities > 95%. To get informations about the chem. purity  
 and possible byproducts or residual solvents the samples were analyzed by  
 HPLC, NMR and GC-MSD. For the last a new technique, the so called solid  
 phase micro extn., SPME was applied for sample prepn. The chem. purity  
 estd. by HPLC anal. was for all CL 20 samples > 96% while the .  
 epsilon.-charge of SNPE had the highest purity (98.3%). From  
 NMR-measurements an acetyl- or formyl-substituted byproduct was  
 identified. From NMR as well as from GC-MSD analyses residual ants. of  
 org. solvents have been detected (ethanol or tetrahydrofuran).  
 Furthermore different spare ants. of other org. components were identified  
 after SPME-treatment and characterization with GC-MSD.  
 IT 135285-90-4, Hexanitrohexaazaisowurtzitane  
 RL: ANT (Analyte); TEM (Technical or engineered material use); ANST  
 (Analytical study); USES (Uses)  
 (anal. characterization of impurities or byproducts in energetic  
 materials by using chromatog. and spectroscopic techniques)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(1minomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-  
 hexanitro- (9CI) (CA INDEX NAME)

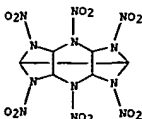


REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 26 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1999:723022 CAPLUS  
 DOCUMENT NUMBER: 131:339087  
 TITLE: Nitration and crystal polymorphism transition in  
 preparation of hexanitrohexaazaisowurtzitane (HNIV)  
 INVENTOR(S): Duddu, Raja; Dave, Paritosh R.  
 PATENT ASSIGNEE(S): USA  
 SOURCE: PCT Int. Appl., 24 pp.  
 CODEN: PIXOD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:  

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9957104	A1	19991111	WO 1999-US9167	19990427
W: AT, AU, BR, CA, CH, CN, DE, DK, ES, FI, GB, IL, JP, KR, LU, MX,				
NO, PT, RU, SE, SG, US, ZA				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,				
PT, SE				
US 6015898	A	20000118	US 1998-71022	19980501
AU 9938697	A1	19991123	AU 1999-38697	19990427
US 6160113	A	20001212	US 1999-300988	19990428
PRIORITY APPLN. INFO.:			US 1998-71022	A 19980501
			WO 1999-US9167	W 19990427

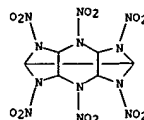
 AB The explosive HNIV (hexanitrohexaazaisowurtzitane) is prepd. by nitration  
 of N-substituted hexaazaisowurtzitane with concd. (i.e., >90%) HNO3 at  
 .gtoreq.75.degree. (preferably 75-115.degree.) in which the substrate  
 contains facile leaving groups selected from .ltoreq.6 H, alkyl, acyl, and  
 acetyl groups, and .ltoreq.2 alkylaryl or NO2 (esp. H, MeCO, HCO, PhCH2,  
 and NO2) groups. A preferred substrate is tetraacetyldiformylisowurtzitan  
 e. The process includes a polymorphic conversion of HNIV product  
 (.alpha.-, .beta.-, and .gamma.-) to the .epsilon.-crystal form  
 comprises prepn. the soln. of HNIV with acetic acid and adding a very  
 small ant. of .epsilon.-HNIV seed crystals, and pptg. .  
 epsilon.-HNIV from the soln.  
 IT 135285-90-4  
 RL: IMP (Industrial manufacture); PUR (Purification or recovery); SPN  
 (Synthetic preparation); PREP (Preparation)  
 (nitration and crystal polymorphism transition in prepn. of  
 hexanitrohexaazaisowurtzitane (HNIV) explosive)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(1minomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-  
 hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS

L10 ANSWER 26 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

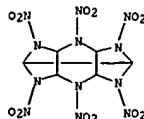
L10 ANSWER 27 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
ACCESSION NUMBER: 1999:454904 CAPLUS  
DOCUMENT NUMBER: 131:118114  
TITLE: Kinetics of thermal decomposition of hexanitrohexaazaisowurtzitane  
AUTHOR(S): Korsounskii, Boris; Nedelko, Vadim; Chukanov, Nikita; Larikova, Tatiana; Volk, Fred  
CORPORATE SOURCE: Institute Chemical Physics Research, Chernogolovka, 142432, Russia  
SOURCE: International Annual Conference of ICT (1999), 30th, 64/1-64/20  
CODEN: IACIEQ; ISSN: 0722-4087  
PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The thermal decompn. of the title compd. (HNIW) in solid state and in soln. was studied by thermo-gravimetry, manometry, optical microscopy, and IR. On linear heating (4 K/min, initial wt. 10 mg), wt. loss of HNIW begins at 235.degree., and self-ignition takes place at 243.degree.. The isothermal decompn. of HNIW in solid state proceeds with a self-acceleration. Kinetics of the reaction is described by the equation of 1st-order autocatalysis. At heating a sample to the exptl. temp., apparently, there is a phase transition .epsiloniln.fvdrw.gamma. whereas during isothermal process no phase transition occurs. On isothermal gravimetric measurements the thermal stability of HNIW is much lower than that of HMX. In m-dinitrobenzene soln. the reaction proceeds according to the 1st-order kinetic equation. The rate consts. and activation parameters of HNIW thermal decompn. in solid state and in soln. were detd. The reactivity of HNIW in soln. exceeds that of HMX by >2 orders. The volatility of HNIW is much lower than that of HMX. N content amts. to approx. 1/2 of gaseous products of HNIW thermolysis. Thermolysis of HNIW and its ignition at heating are accompanied by formation of a condensed residue. During these processes 5 of 6 NO2 groups present in a HNIW mol. are lost. The residue contains NH2 groups and does not contain C-H bonds.  
IT 135285-90-4, Hexanitrohexaazaisowurtzitane  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)  
(thermal decompn. of nitrohexaazaisowurtzitane and kinetics thereof)  
RN 135285-90-4 CAPLUS  
CN 5,2,6-(1aminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS

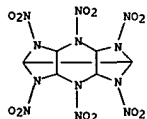
L10 ANSWER 27 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 28 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
ACCESSION NUMBER: 1999:273151 CAPLUS  
DOCUMENT NUMBER: 131:18700  
TITLE: Effect of particle size on the thermal decomposition of .vepsiln.-hexanitrohexaazaisowurtzitane  
AUTHOR(S): Kim, Jun-Hyung; Yim, Yoo-Jin  
CORPORATE SOURCE: Agency for Defense Development, Taejon, 305-600, S. Korea  
SOURCE: Journal of Chemical Engineering of Japan (1999), 32(2), 237-241  
CODEN: JCEJAJ; ISSN: 0021-9592  
PUBLISHER: Society of Chemical Engineers, Japan  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The influence of the particle size on the thermal decompn. of .epsiloniln.-hexanitrohexaazaisowurtzitane (HNIW) was studied by DSC. The kinetics and mechanism for the decompn. were evaluated using integral methods. The thermal kinetic parameters such as activation energy (E) and pre-exponential factor (A) depend little on the particle size of .epsiloniln.-HNIW in the range 4-180 .mu.m, and an A3 model function fits most of the data from the decompn. of the material.  
IT 135285-90-4, Hexanitrohexaazaisowurtzitane  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)  
(effect of particle size on thermal decompn. of .vepsiln.-hexanitrohexaazaisowurtzitane)  
RN 135285-90-4 CAPLUS  
CN 5,2,6-(1aminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)

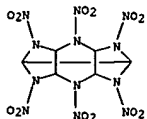


REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

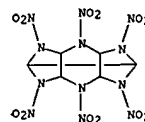
**110 ANSWER 29 OF 47** CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1998:498910 CAPLUS  
 DOCUMENT NUMBER: 129:110975  
 TITLE: Characterization of impurities in new energetic materials  
 AUTHOR(S): Bunte, G.; Pontius, H.; Kaiser, M.  
 CORPORATE SOURCE: Fraunhofer-Inst. Chemische Technologie, Pfinztal, D-76327, Germany  
 SOURCE: International Annual Conference of ICT (1998), 29th(Energetic Materials), 148.1-148.10  
 CODEN: IACIEQ; ISSN: 0722-4087  
 PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Three samples of hexanitrohexaazaisowurtzitane (HNHW, CL 20) from different suppliers (.epsilon.-CL 20 from Thiokol, USA and .epsilon.- and .beta.- CL 20 from SNPE, France) were analyzed with chromatog. and spectroscopic techniques to characterize the chem. and polymorph purity of the materials to compare the different samples. IR-spectroscopic measurements showed that all 3 materials have polymorph purities >95 %. To get information about the chem. purity and possible byproducts or residual solvents the samples were analyzed by HPLC, NMR, and GC-MSD. Solid-Phase Micro Extn. (SPME) was applied for sample prep. The chem. purity estd. by HPLC anal. was for all CL 20 samples >96 % while the .epsilon.-charge of SNPE had the highest purity (98.3%). From NMR-measurements a formyl-substituted byproduct was identified. From NMR as well as from GC-MSD analyses residual ants. of org. solvents were detected (ethanol or tetrahydrofurane). Furthermore different spare ants. of other org. components were identified after SPME-treatment and characterization with GC-MSD.  
 IT 135285-90-4, CL 20  
 RL: AMX (Analytical matrix); TEM (Technical or engineered material use); ANST (Analytical study); USES (Uses)  
 (anal. characterization of impurities in)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(1minomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



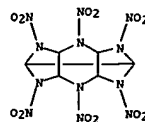
**110 ANSWER 31 OF 47** CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1998:498855 CAPLUS  
 DOCUMENT NUMBER: 129:138140  
 TITLE: Fine grinding of explosives  
 AUTHOR(S): Gerber, P.; Zilly, B.; Teipel, U.  
 CORPORATE SOURCE: Fraunhofer-Institut Chemische Technologie, Pfinztal, D-76327, Germany  
 SOURCE: International Annual Conference of ICT (1998), 29th(Energetic Materials), 71.1-71.12  
 CODEN: IACIEQ; ISSN: 0722-4087  
 PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 AB A wet grinding process with a rotor-stator mill was selected for safe grinding of the explosive .epsilon.-CL-20 with a mean particle size of 200 .mu.m to produce a narrow particle size distribution and a mean particle size of 5 .mu.m. The aq. suspension had a solid concn. of 15%. The obtained particle size distribution of .epsilon.-CL-20 is compared to that of RDX.  
 IT 135285-90-4, CL-20  
 RL: PEP (Physical, engineering or chemical process); FRP (Properties); TEM (Technical or engineered material use); PROC (Process); USES (Uses)  
 (fine grinding of explosives)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(1minomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



**110 ANSWER 30 OF 47** CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1998:498907 CAPLUS  
 DOCUMENT NUMBER: 129:138146  
 TITLE: Thermal behavior and stability of HNHW (CL20)  
 AUTHOR(S): Loebbecke, S.; Bohn, M. A.; Pfeil, A.; Krause, A.  
 CORPORATE SOURCE: Fraunhofer-Inst. Chemische Technologie, Pfinztal, D-76318, Germany  
 SOURCE: International Annual Conference of ICT (1998), 29th(Energetic Materials), 145.1-145.15  
 CODEN: IACIEQ; ISSN: 0722-4087  
 PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The thermal stability, phase behavior, and decompn. of the explosive .epsilon.-2,4,6,8,10,12-hexanitrohexaazaisowurtzitane (HNHW) were studied. At >164.degree. irreversible transition to the .gamma.-polymorph was obsd. which is accompanied by an increase of vol. Differential scanning calorimetry and differential thermogravimetry indicate a 2-step decompn. at >210.degree.. The evolution of gaseous decompn. products was monitored by rapid scan FTIR spectroscopy. The main products are CO2, NO2, H2O, and HCN. In addn., a solid residue remains whose IR spectrum is given. A mass loss due to decompn. was also obsd. below 210.degree.. Kinetic calcs. show this low-temp. decompn. reaction to be of 1st order and autocatalytic.  
 IT 135285-90-4, CL-20  
 RL: PEP (Physical, engineering or chemical process); FRP (Properties); TEM (Technical or engineered material use); PROC (Process); USES (Uses)  
 (thermal behavior and stability of HNHW (CL 20))  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(1minomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



**110 ANSWER 32 OF 47** CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1998:60143 CAPLUS  
 DOCUMENT NUMBER: 128:117010  
 TITLE: Sensitivity and spectroscopic properties of the .beta.- and .epsilon.-polymorphs of HNHW  
 AUTHOR(S): Ostmark, Henrik; Bergman, Helena; Sjöberg, Per  
 CORPORATE SOURCE: Natl. Defence Res. Establishment, Sundbyberg, S-172 90, Swed.  
 SOURCE: Proceedings - International Symposium on Energetic Materials Technology, Phoenix, 1995 (1995), 76-81.  
 American Defense Preparedness Association: Arlington, Va.  
 CODEN: 65NDAP  
 DOCUMENT TYPE: Conference  
 LANGUAGE: English  
 AB A study was presented of the sensitivity and spectroscopic properties of the .beta.- and .epsilon.-polymorphs of HNHW (2,4,6,8,10,12-hexanitrohexaazaisowurtzitane). The thermal stability was studied using DSC technique which was also used to measure the activation energy and the frequency factor. The sensitivity was examd. by drop-wt. test and friction test. The drop-wt. test points to a higher sensitivity for the .epsilon.-polymorph (18 cm for .epsilon.- vs. 67 cm for the .beta.-polymorph), whereas the sensitivity to friction was similar for the two polymorphs. A HPLC anal. method was developed to analyze HNHW in soln. Mass spectra (electron impact and chem. ionization) for both polymorphs were also given. The best routine method so far for analyzing the polymorphs of HNHW is Fourier-transform IR spectroscopy which was used to distinguish the polymorphs. An alternative to the FTIR method, Fourier-transform Raman spectroscopy (FT Raman spectroscopy), uses only a small amt. of solid samples (a few mg) and was easy to carry out. The FT Raman spectra for the .beta.- and .epsilon.-polymorphs of HNHW showed major differences and can thus be used for fingerprinting.  
 IT 135285-90-4  
 RL: FRP (Properties); TEM (Technical or engineered material use); USES (Uses)  
 (sensitivity and spectroscopic properties of .beta.- and .epsilon.-polymorphs of HNHW)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(1minomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



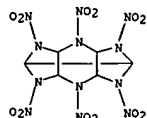
10 ANSWER 33 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1998:38963 CAPLUS  
 DOCUMENT NUMBER: 128:121916

TITLE: Molecular Packing and NPT-Molecular Dynamics Investigation of the Transferability of the RDX Inter-molecular Potential to 2,4,6,8,10,12-Hexanitrohexaazaisowurtzitane  
 AUTHOR(S): Soreacu, Dan C.; Rice, Betsy M.; Thompson, Donald L.  
 CORPORATE SOURCE: Department of Chemistry, Oklahoma State University, Stillwater, OK, 74078, USA  
 SOURCE: Journal of Physical Chemistry B (1998), 102(6), 948-952  
 CODEN: JPCBFX; ISSN: 1089-5647

PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The degree to which an intermol. potential for the explosive hexahydro-1,3,5-trinitro-1,3,5-s-triazine (RDX) is transferable for predictions of crystal structures (within the approxn. of rigid mols.) of a similar chem. system, in this case, polymorphic phases of the 2,4,6,8,10,12-hexanitrohexaazaisowurtzitane (HNW) crystal was explored. Mol. packing and isothermal-isobaric mol. dynamics calcn. performed with this potential reproduce the main crystallog. features of the .epsilon.-, .beta.-, and .gamma.-HNW crystals. Thermal expansion coeffs. calcd. using the present model predict near isotropic expansion for the .epsilon.- and .gamma.-HNW crystals phases and anisotropic expansion for .beta.-HNW.  
 IT 135285-90-4, 2,4,6,8,10,12-Hexanitrohexaazaisowurtzitane  
 RL: PRP (Properties)

(mol. packing and NPT-mol. dynamics investigation of transferability of RDX intermol. potential to calcn. of crystal structure of hexanitrohexaazaisowurtzitane)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

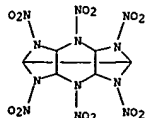
10 ANSWER 35 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1997:570534 CAPLUS  
 DOCUMENT NUMBER: 127:236415

TITLE: Theoretical calculation on .epsilon.-Hexanitrohexaazaisowurtzitane structure  
 AUTHOR(S): Li, Laicai; Yang, Chun  
 CORPORATE SOURCE: Department of Chemistry, Sichuan Normal University, Chengdu, 610066, Peop. Rep. China  
 SOURCE: Sichuan Shifan Daxue Xuebao, Ziran Kexueban (1997), 20(3), 71-73  
 CODEN: SKXEEF; ISSN: 1001-8395

PUBLISHER: Sichuan Shifan Daxue  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Chinese

AB The PM3 (MO) method was used to optimize the structure of .epsilon.-HNW (hexanitrohexaazaisowurtzitane), and the explosive properties of .epsilon.-HNW were discussed theor.  
 IT 135285-90-4  
 RL: PRP (Properties)

(PM3 MO calcn. of structure and properties of .epsilon.-HNW)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



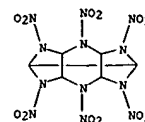
10 ANSWER 34 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1997:730088 CAPLUS  
 DOCUMENT NUMBER: 128:5410

TITLE: CL-20 performance exceeds that of HMX and its sensitivity is moderate  
 AUTHOR(S): Simpson, R. L.; Urtiew, P. A.; Ornellas, D. L.; Moody, G. L.; Scribner, K. J.; Hoffmann, D. M.  
 CORPORATE SOURCE: Energetic Materials Center, University California, Livermore, CA, 94550, USA  
 SOURCE: Propellants, Explosives, Pyrotechnics (1997), 22(5), 249-255  
 CODEN: PEPYD5; ISSN: 0721-3115

PUBLISHER: Wiley-VCH Verlag GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The explosive performance of .epsilon.-CL-20 is approx. 14% greater than that of HMX as detd. by cylinder expansion and Ta plate acceleration expts. This makes it the most powerful explosive ever tested at small vol. expansions of the detonation products. In general CL-20 is more sensitive than HMX. However, the sensitivity of CL-20 to 1-dimensional shock loading is similar to HMX.  
 IT 135285-90-4, CL 20  
 RL: PRP (Properties)

(explosive performance and sensitivity of CL-20 compared with HMX)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



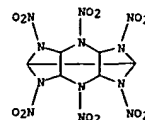
10 ANSWER 36 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1996:517341 CAPLUS  
 DOCUMENT NUMBER: 125:200045

TITLE: Shock initiation of an .epsilon.-CL-20-Estane formulation  
 AUTHOR(S): Tarver, C. M.; Simpson, R. L.; Urtiew, P. A.  
 CORPORATE SOURCE: Lawrence Livermore National Laboratory, Livermore, CA, 94551, USA  
 SOURCE: AIP Conference Proceedings (1996), 370(Pt. 2, Shock Compression of Condensed Matter--1995), 891-894  
 CODEN: APCPCS; ISSN: 0094-243X

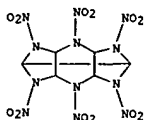
PUBLISHER: AIP Press  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The shock sensitivity of a pressed solid explosive formulation, LX-19, contg. 95.2% by wt. .epsilon.-phase 2,4,6,8,10,12-hexanitrohexaazaisowurtzitane (HNW) and 4.8% Estane binder, was detd. using the wedge test and embedded manganin pressure gauge techniques. This formulation was slightly more sensitive than LX-14, which contains 95.5% HMX and 4.5% Estane binder. The measured pressure histories for LX-19 were very similar to those obtained using several HMX-inert binder formulations. An ignition and growth reactive flow model for LX-19 was developed (using two Jones-Wilkins-Lee equations of state) which differed from those for HMX-inert binder formulations only by a 25% higher hot spot growth rate.  
 IT 135285-90-4, LX 19  
 RL: RCT (Reactant); TEM (Technical or engineered material use); RACT (Reactant or reagent); USES (Uses)

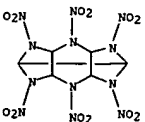
(LX 19: flow modeling of shock sensitivity of pressed explosive contg. hexanitrohexaazaisowurtzitane and estane binder)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



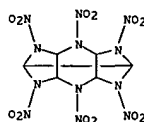
ANSWER 37 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1996:470483 CAPLUS  
 DOCUMENT NUMBER: 125:128340  
 TITLE: Crystal and molecular structures of .epsilon.-HNIW  
 AUTHOR(S): Zhao, Xinqi; Shi, Nicheng  
 CORPORATE SOURCE: Department Chemical Engineering, Beijing Institute Technology, Beijing, 100081, Peop. Rep. China  
 SOURCE: Chinese Science Bulletin (1996), 41(7), 574-576  
 CODEN: CSBUEF; ISSN: 1001-6538  
 PUBLISHER: Science Press  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The title compd. (the polymorph of hexanitrohexaazaisowurtzitane with the highest crystal d.) is monoclinic, space group P21/a, with a 1.3696(7), b 1.2554(6), c 0.8833(4) nm, and .beta. 111.18(2).degree.; Z = 4, dc = 2.055; R = 0.066, Rw = 0.074 for 2658 reflections. At. coordinates are given. The C-N and C-H bond lengths in the mol. are typical. The nitramine group is essentially in a plane configuration. C-C bond lengths are 0.1575-0.1590 nm.  
 IT 135285-90-4, Hexanitrohexaazaisowurtzitane  
 RL: PRP (Properties)  
 (crystal structure of polymorph of)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



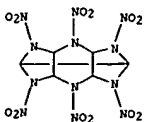
ANSWER 39 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1996:285182 CAPLUS  
 DOCUMENT NUMBER: 124:320934  
 TITLE: Study on 100.degree.C heat test of .epsilon.-HNIW  
 AUTHOR(S): Zhao, Xinqi; Li, Li; Yang, Zongyun; Yu, Yongzhong  
 CORPORATE SOURCE: Beijing Institute Technology, Beijing, 100081, Peop. Rep. China  
 SOURCE: Proceedings of the Beijing International Symposium on Pyrotechnics and Explosives, 3rd, Beijing, Nov. 6-9, 1995 (1995), 312-314. Editor(s): Yuxiang, Ou. China Ordnance Society: Beijing, Peop. Rep. China.  
 CODEN: 62RIAT  
 DOCUMENT TYPE: Conference  
 LANGUAGE: English  
 AB Loss in wt. of .epsilon.-HNIW (CL-20) at 100.degree. during two 48-h periods was only 0.02%, and no changes in phys. appearance of the crystals were noted. Neither ignition nor explosion occurred after 300-h heating. The FTIR spectra before and after 300-h heating confirmed that no phase transformation was evident.  
 IT 135285-90-4, Hexanitrohexaazaisowurtzitane  
 RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)  
 (explosive; thermal stability of)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



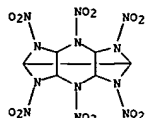
ANSWER 38 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1996:285210 CAPLUS  
 DOCUMENT NUMBER: 124:320936  
 TITLE: Determination of thermal stabilities of .epsilon.-CL-20 and HMX using accelerating rate calorimeter (ARC)  
 AUTHOR(S): Van, Xingzhong; Ou, Yuxiang; Chen, Boron; Feng, Changgen  
 CORPORATE SOURCE: Beijing Institute Technology, Beijing, 100081, Peop. Rep. China  
 SOURCE: Proceedings of the Beijing International Symposium on Pyrotechnics and Explosives, 3rd, Beijing, Nov. 6-9, 1995 (1995), 520-525. Editor(s): Yuxiang, Ou. China Ordnance Society: Beijing, Peop. Rep. China.  
 CODEN: 62RIAT  
 DOCUMENT TYPE: Conference  
 LANGUAGE: English  
 AB The adiabatic thermal decompn. kinetics of .epsilon.-CL-20 and HMX was studied in an accelerating rate calorimeter. The self-heating rates and the pressure increase rates were measured as function of self-heating temp. The activation energies for the decompn. of these explosives were detd. from the self-heating rates. The onset temp. of the self-heating was always much lower than the corresponding std. deflagration temp. (which was detd. with a std. app.). The temp. of onset of self-heating of .epsilon.-CL-20 was lower than that of HMX.  
 IT 135285-90-4  
 RL: PRP (Properties)  
 (thermal stability and adiabatic thermal decompn. kinetics of HNIW and HMX in accelerating rate calorimeter)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



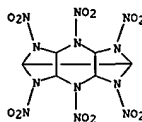
ANSWER 40 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1996:255293 CAPLUS  
 DOCUMENT NUMBER: 124:293607  
 TITLE: Phase transition in HNIW (CL-20) polymorphs and its application in propellants  
 AUTHOR(S): Feng, Zengguo  
 CORPORATE SOURCE: Beijing Inst. of Technology, Beijing, 100081, Peop. Rep. China  
 SOURCE: Binggong Xuebao, Huohuangong Fence (1996), 18(1), 46-9, 42  
 CODEN: EXHFFP; ISSN: 1004-9193  
 PUBLISHER: Zhongguo Bingqi Gongye Di-204 Yanjiusuo  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Chinese  
 AB Recently, hexanitrohexaazaisowurtzitane (HNIW; i.e. CL-20) was obsd. to exist in six different polymorphs, from which .alpha., .beta., .gamma., and .epsilon.-polymorphs have been sepd. and detd. Calcns. for detonation parameters and specific impulse revealed that CL-20 was more energetic than HMX and RDX, but it was remarkably different with respect to phase conversion, thermal stability, and soly. Based on available refs. and exptl. data on RDX and polymorphic changes of ammonium nitrate, some views were suggested about phase transitions in CL-20 polymorphs and its application in propellants.  
 IT 135285-90-4  
 RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)  
 (phase transition in HNIW polymorphs and application as solid propellants)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



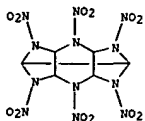
**ANSWER 41 OF 47** CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1996:202406 CAPLUS  
 DOCUMENT NUMBER: 124:236477  
 TITLE: Thermal stability of .epsilon.-HNHAIW at 100.degree.C  
 AUTHOR(S): Zhao, Xinqi; Li, Li  
 CORPORATE SOURCE: Sch. Chem. Eng. Materials Sci., Beijing Inst. Technol., Beijing, 100081, Peop. Rep. China  
 SOURCE: Hanneng Cailliao (1995), 3(4), 31-4  
 CODEN: HACAPO; ISSN: 1006-9941  
 PUBLISHER: Hanneng Cailliao Bianjibu  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Chinese  
 AB Hexanitrohexaazaisowurtzitane (HNHAIW) was heated at 100.degree. for 48.96 and 300 h, resp., with no observable burning or explosion. The crystals had no visible changes in appearance and no crystal configuration transitions identifiable by FT-IR anal. A wt. loss of 0.02% after 96 h heating indicated that the thermal stability of .epsilon.-HNHAIW was better than that of RDX and HMX.  
 IT 135285-90-4, Hexanitrohexaazaisowurtzitane  
 RL: PRP (Properties)  
 (thermal stability of)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



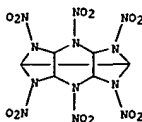
**ANSWER 42 OF 47** CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1995:985376 CAPLUS  
 DOCUMENT NUMBER: 124:33113  
 TITLE: Structural identification of hexanitrohexaazaisowurtzitane  
 AUTHOR(S): Ou, Yuxiang; Chen, Boren; Jia, Huiping; Fan, Zelin; Xu, Yongjiang  
 CORPORATE SOURCE: College Chem. Eng. Material Sci., Beijing Inst. Technology, Beijing, 100081, Peop. Rep. China  
 SOURCE: Hanneng Cailliao (1995), 3(3), 1-8  
 CODEN: HACAPO; ISSN: 1006-9941  
 PUBLISHER: Hanneng Cailliao Bianjibu  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Chinese  
 AB The mol. structure of CL-20 synthesized by authors was identified by FTIR, 1H-NMR, 13C-NMR, CIMS, UV, and elemental anal. The four polymorphs (.alpha., .beta., .gamma., and .epsilon.) of CL-20 was prepd., and also characterized by FTIR. The characteristic peaks of the polymorphs in the "fingerprint" region (1200-700 cm-1) were in agreement with those reported in literatures. The structure of CL-20 and its four polymorphs were clarified.  
 IT 135285-90-4P, Hexanitrohexaazaisowurtzitane  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (structural identification of hexanitrohexaazaisowurtzitane and its polymorphs)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



**ANSWER 43 OF 47** CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1995:507758 CAPLUS  
 DOCUMENT NUMBER: 123:36618  
 TITLE: Sensitivity studies of a new energetic formulation  
 AUTHOR(S): Wilson, W. H.; Forbes, J. W.; Liddiard, T. P.; Doherty, R. M.  
 CORPORATE SOURCE: Dahlgren Div., Naval Surface Warfare Cent., Silver Spring, MD, 20903-5640, USA  
 SOURCE: AIP Conference Proceedings (1994), 309(High-Pressure Science and Technology--1993, Pt. 2), 1401-4  
 CODEN: APCPCS; ISSN: 0094-243X  
 PUBLISHER: AIP Press  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The shock sensitivity of a new pressed formulation, PEXC 19, which is similar to LX-14 but contains CL-20 instead of HMX, was studied. Samples were made from a bimodal particle size distribution of CL-20 .epsilon.-polymorph and an ethylene-vinyl acetate binder, pressed to an av. 97% of theor. max. d. The material exhibited an anomalous reversal in slope of shock sensitivity vs. input stress. Over a limited stress range near the first reaction threshold, the level of reaction decreased with increasing input stress. Within this range of input shock, it was obsd. that break-off of reaction was delayed, and was concd. near the sample centerline.  
 IT 135285-90-4, CL-20  
 RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)  
 (explosives contg.; shock sensitivity of pressed CL20-based explosive formulation)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



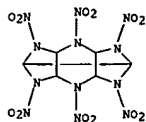
**ANSWER 44 OF 47** CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1994:438726 CAPLUS  
 DOCUMENT NUMBER: 121:38726  
 TITLE: The thermal stability of the polymorphs of hexanitrohexaazaisowurtzitane. Part II  
 AUTHOR(S): Foltz, M. Frances; Coon, Clifford L.; Garcia, Frank; Nichols, Albert L., III  
 CORPORATE SOURCE: Lawrence Livermore Natl. Lab., Livermore, CA, 94550, USA  
 SOURCE: Propellants, Explosives, Pyrotechnics (1994), 19(3), 133-44  
 CODEN: PEPYDS; ISSN: 0721-3115  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Solid-solid phase transitions in the .alpha.-, .beta.-, .gamma.-, and .epsilon.-polymorphs of 2,4,6,8,10,12-hexanitrohexaazaisowurtzitane (HNW) were studied as a function of temp. Techniques used include differential scanning calorimetry (DSC), DTA/thermogravimetric anal. (DTA/TGA), and hot stage microscope anal. Fourier-transform IR spectroscopy (FTIR) was used to identify results of polymorphic conversion. Results corroborate those of Part I [M. Foltz, C. Coon, et al (1994)] that the existence of multiple .alpha.-hydrate phases complicates definition of the HNHW pressure-temp. phase diagram. A high-temp. endothermic DSC response was detd. by FTIR spectroscopy to be the .beta.- to .gamma. transition, not a conversion to a high-temp. "delta" phase. The role of water in the shifting this conversion to higher temp. was discussed.  
 IT 135285-90-4  
 RL: USES (Uses)  
 (polymorphs of, thermal stability of)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



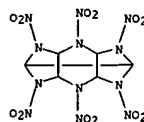


10/042,522

10 ANSWER 45 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1994:326923 CAPLUS  
 DOCUMENT NUMBER: 120:326923  
 TITLE: Thermal stability of .epsilon.-hexanitrohexaazaisowurtzitane in an Estane formulation  
 AUTHOR(S): Foltz, M. Frances  
 CORPORATE SOURCE: Lawrence Livermore Natl. Lab., Livermore, CA, 94550, USA  
 SOURCE: Propellants, Explosives, Pyrotechnics (1994), 19(2), 63-9  
 CODEN: PEPYD5; ISSN: 0721-3115  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A change in color and d. during prolonged heating of a formulation contg. .epsilon.-hexanitrohexaazaisowurtzitane (HNIW) and Estane 5702 was investigated by Fourier transform IR spectroscopy. Polymorphic impurities were obsd. at all stages of prodn. and processing, the nature and concn. of which changed with treatment of the material. Thermally-induced polymorphic conversion was detd. to be the cause of the decrease in d., whereas the color change was speculated to be the result of binder degradn. Sensitivity to impact, friction, and electrostatic spark were unchanged.  
 IT 135285-90-4, Hexanitrohexaazaisowurtzitane  
 RL: USES (Uses)  
 (explosives, contg. urethane rubber binder, thermal stability of)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(1minomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



10 ANSWER 46 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1994:248721 CAPLUS  
 DOCUMENT NUMBER: 120:248721  
 TITLE: The thermal stability of the polymorphs of hexanitrohexaazaisowurtzitane. Part I  
 AUTHOR(S): Foltz, M. Frances; Coon, Clifford L.; Garcia, Frank; Nicholas, Albert L., III  
 CORPORATE SOURCE: Lawrence Livermore Natl. Lab., Livermore, CA, 94550, USA  
 SOURCE: Propellants, Explosives, Pyrotechnics (1994), 19(1), 19-25  
 CODEN: PEPYD5; ISSN: 0721-3115  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Phase transitions in the .alpha.-, .beta.-, .gamma.-, and .epsilon.-polymorphs of 2,4,6,8,10,12-hexanitrohexaazaisowurtzitane (HNIW) were studied as a function of temp. In addn., results were presented for high-temp. equil. solvation studies coupled with Fourier-transform IR spectroscopy for the identification of polymorphic conversion. These results were augmented by literature data from differential scanning calorimetry, DTA-thermogravimetric anal., and optical hot-stage microscopy. The thermodyn. stability of the polymorphs decreased in the order .epsilon. > .gamma. > .alpha.-hydrate > .beta., with the .epsilon. polymorph being the most thermodynamically stable phase of HNIW at room temp. The existence of multiple .alpha.-hydrate phases complicated the detn. of the equil. pressure-temp. phase diagram of HNIW.  
 IT 135285-90-4  
 RL: USES (Uses)  
 (polymorphs of, phase transitions and thermal anal. and phase diagrams of)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(1minomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



10 ANSWER 47 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1993:132609 CAPLUS  
 DOCUMENT NUMBER: 118:132609  
 TITLE: Pressure/temperature phase diagram of hexanitrohexaazaisowurtzitane  
 AUTHOR(S): Russell, T. P.; Miller, P. J.; Piermarini, G. J.; Block, S.  
 CORPORATE SOURCE: Nav. Surface Warfare Cent., Silver Spring, MD, 20901-5000, USA  
 SOURCE: Journal of Physical Chemistry (1993), 97(9), 1993-7  
 CODEN: JPCHAX; ISSN: 0022-3654  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The five known polymorphs of hexanitrohexaazaisowurtzitane (chem. name: 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazatetracyclo[5.5.0.0.0.5.9.03.11] dodecane), .alpha.-, .beta.-, .gamma.-, .epsilon.-, and .zeta.-, were studied by optical polarizing light microscopy (OPLM) and Fourier transform IR spectroscopy (FTIR) as a function of temp. and pressure. A high-temperature/high-pressure diamond anvil cell specially designed for these studies was employed. Four reversible and five unidirectional phase transformations were obsd. and identified by FTIR spectra. Phase boundaries were studied as a function of pressure and temp. permitting a delineation of the various polymorph stability fields. A pressure/temp. reaction/phase diagram for the .gamma. polymorph to 14.0 GPa and temps. between -125 and 340 degree. (or to thermal decompn. temps.), is presented. The FTIR spectra for all five polymorphs were obtained as functions of temp. and pressure. An .alpha. phase with trapped CO2/CO was obsd. by FTIR. The thermal decompn. temp./pressure parameters were also detd.  
 IT 135285-90-4  
 RL: PRP (Properties)  
 (pressure-temp. phase diagram of)  
 RN 135285-90-4 CAPLUS  
 CN 5,2,6-(1minomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)

